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Excess Molar Enthalpies of Acetophenone + (Methanol, + Ethanol, + 1-Propanol, and + 2-Propanol) at Different Temperatures and Pressures

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Excess molar enthalpies of four binary systems for acetophenone + (methanol, + ethanol, + 1-propanol, and + 2-propanol) at T = (298.15, 313.15, 328.15, 338.15, and 348.15) K and p = (0.1 and 10.0) MPa were determined by a high-pressure flow-mixing isothermal microcalorimeter. The excess molar enthalpies increased with an increase in the temperature, pressure, and the molecular size of alcohols. The experimental data were correlated by the Redlich–Kister equation and three local composition models (Wilson, NRTL, and UNIQUAC).

Introduction

Acetophenone, as an important industrial chemical and is widely used as ingredients of flavor and fragrance in soaps, detergents, cosmetics, and perfumes. It has also been used as an important intermediate for pharmaceuticals and agrochemicals.

The thermodynamic properties of systems containing acetophenone are helpful to better understand molecular interaction and to design and simulate the different processes of separation. The properties of pure acetophone have been studied with the help of experiment[1,2] and theoretical analysis.[3] The excess molar enthalpies of mixtures are fundamental thermodynamic data, e.g., a correct description of the temperature dependence of activity coefficients following the Gibbs–Helmholtz equation

$$\left(\frac{\partial \ln \gamma_i}{\partial 1/T}\right)_{p,x} = \frac{H_i^{\mathrm{E}}}{R} \tag{1}$$

Until now, very limited data of excess molar enthalpies of systems containing acetophenone could be found in the literature.[4–6] In this paper, the excess molar enthalpies of four binary systems for acetophenone + (methanol, + ethanol, + 1-propanol, and + 2-propanol) were determined using a high-pressure flow-mixing isothermal microcalorimeter at T = (298.15, 313.15, 328.15, 338.15, and 348.15) K and p = (0.1 and 10.0) MPa. The experimental data were correlated using the Redlich–Kister equation and three local composition models: the Wilson model, the NRTL model, and the UNIQUAC model.

Table 1. Excess Molar Enthalpies of the System Acetophenone (1) + Methanol (2)

x_1	H_m^E/J·mol^{-1}	x_1	H_m^E/J·mol^{-1}	x_1	H_m^E/J·mol^{-1}
T = 298.15 K, p = 0.1 MPa					
0.0999	363.7	0.4001	876.5	0.5995	912.7
0.1999	613.5	0.4496	905.4	0.6992	841.0
0.2997	775.5	0.4998	921.1	0.7990	681.7
0.3506	833.7	0.5500	924.2	0.9003	403.7
T = 298.15 K, p = 10.0 MPa					
0.0997	373.6	0.3996	898.8	0.5990	944.1
0.1996	623.9	0.4491	929.9	0.6988	871.5
0.2993	793.4	0.4993	947.5	0.7986	715.8
0.3501	855.9	0.5495	953.1	0.9001	435.0
T = 313.15 K, p = 0.1 MPa					
0.0999	410.2	0.4001	1023.3	0.5995	1099.1
0.1999	696.2	0.4496	1061.1	0.6992	1013.3
0.2997	897.4	0.4998	1087.0	0.7990	819.0
0.3506	970.4	0.5500	1101.5	0.9003	493.7
T = 313.15 K, p = 10.0 MPa					
0.0997	427.7	0.3996	1054.1	0.5990	1101.9
0.1996	723.7	0.4491	1090.7	0.6988	1016.8
0.2993	925.9	0.4993	1109.8	0.7986	823.6
0.3501	1000.6	0.5495	1112.0	0.9001	496.6
T = 328.15 K, p = 0.1 MPa					
0.0999	480.2	0.4001	1171.4	0.5995	1218.5
0.1999	802.7	0.4496	1211.5	0.6992	1109.1
0.2997	1024.3	0.4998	1233.5	0.7990	876.4
0.3506	1109.3	0.5500	1235.9	0.9003	502.0
T = 328.15 K, p = 10.0 MPa					
0.0997	482.1	0.3996	1174.2	0.5990	1222.1
0.1996	809.6	0.4491	1214.2	0.6988	1110.3
0.2993	1030.7	0.4993	1235.5	0.7986	877.5
0.3501	1114.6	0.5495	1239.8	0.9001	503.7

Experimental Section

Materials. Acetophenone (guaranteed grade, w = 0.998) was purchased from Shanghai Jiachen Chemical Co., Ltd. Methanol, ethanol, 1-propanol, and 2-propanol (HPLC, w = 0.997) were provided by Tianjin Saifu Technologies Co., Ltd. and dried with molecular sieves (3 to 4) Å. The mass fraction purities of these compounds were determined by gas chromatography to be greater than w = 0.998. Before use, all chemicals were degassed by evacuation.

Apparatus and Procedure. A commercial isothermal microcalorimeter (model IMC 4400, Calorimetry Sciences Corporation, USA) with a refrigerating/heating circulator (model 9000, PolyScience Inc., USA) was used. The flow-mixing system was comprised of a sample cell and a reference cell (model CSC 4442), two syringe pumps (model 260D, ISCO Inc., USA), and a back-pressure regulator (model CSC 4448). The IMC data acquisition software was provided by Calorimeter Science

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Table 2. Excess Molar Enthalpies of the System Acetophenone (1) + Ethanol (2)

x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$	x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$	x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$
$T = 298.15$ K, $p = 0.1$ MPa					
0.1003	480.5	0.4009	1123.8	0.5998	1157.4
0.2002	790.9	0.4504	1158.7	0.7002	1062.9
0.3006	999.5	0.5007	1177.4	0.7996	868.4
0.3500	1069.9	0.5502	1176.8	0.9002	527.5
$T = 298.15$ K, $p = 10.0$ MPa					
0.1002	484.9	0.4006	1125.2	0.5995	1164.4
0.2000	792.5	0.4501	1159.4	0.6999	1074.1
0.3004	1000.6	0.5004	1178.8	0.7995	887.5
0.3498	1071.2	0.5499	1179.3	0.9001	541.8
$T = 313.15$ K, $p = 0.1$ MPa					
0.1003	557.9	0.4009	1328.6	0.5998	1377.7
0.2002	932.4	0.4504	1369.5	0.7002	1258.6
0.3006	1184.0	0.5007	1391.6	0.7996	1021.5
0.3500	1270.5	0.5502	1397.2	0.9002	608.5
$T = 313.15$ K, $p = 10.00$ MPa					
0.1002	559.1	0.4006	1330.7	0.5995	1378.4
0.2000	933.3	0.4501	1370.1	0.6999	1261.5
0.3004	1184.3	0.5004	1392.8	0.7995	1021.9
0.3498	1271.6	0.5499	1399.4	0.9001	609.7
$T = 328.15$ K, $p = 0.1$ MPa					
0.1003	612.3	0.4009	1497.6	0.5998	1527.5
0.2002	1036.9	0.4504	1544.3	0.7002	1375.5
0.3006	1328.9	0.5007	1565.2	0.7996	1081.9
0.3500	1425.4	0.5502	1559.8	0.9002	630.0
$T = 328.15$ K, $p = 10.0$ MPa					
0.1002	613.3	0.4006	1498.0	0.5995	1530.1
0.2000	1037.7	0.4501	1545.7	0.6999	1380.0
0.3004	1329.3	0.5004	1567.1	0.7995	1094.3
0.3498	1425.8	0.5499	1561.1	0.9001	635.6
$T = 338.15$ K, $p = 0.1$ MPa					
0.1003	670.3	0.4009	1608.2	0.5998	1614.3
0.2002	1122.8	0.4504	1651.8	0.7002	1437.5
0.3006	1430.6	0.5007	1669.4	0.7996	1119.7
0.3500	1534.1	0.5502	1657.3	0.9002	636.1
$T = 338.15$ K, $p = 10.0$ MPa					
0.1002	671.7	0.4006	1610.2	0.5995	1616.4
0.2000	1122.9	0.4501	1653.0	0.6999	1440.9
0.3004	1431.8	0.5004	1671.4	0.7995	1123.5
0.3498	1535.2	0.5499	1658.2	0.9001	639.6

Corporation. The uncertainty of composition on mole fraction basis was 0.0005. The uncertainties of the temperature and pressure were 0.1 K and 0.1 kPa, respectively. The uncertainty of H_m^E value was less than 1.0 %. The experimental procedure and the reliability of the apparatus have been described in detail elsewhere.[7]

Results and Discussion

In this work, the excess molar enthalpies of four binary systems for acetophenone + (methanol, + ethanol, + 1-propanol, and + 2-propanol) have been measured at $T = (298.15, 313.15, 328.15, 338.15, \text{and } 348.15)$ K and $p = (0.1 \text{ and } 10.0)$ MPa. The experimental data are listed in Tables 1 to 4. As examples, excess molar enthalpies of acetophenone (1) + methanol (2) in Table 1 and acetophenone (1) + alcohols (2) at 298.15 K and 0.1 MPa are plotted in Figures 1 and 2, respectively.

The experimental data of excess molar enthalpies are correlated by the Redlich–Kister equation and three local composition models (Wilson, NRTL, and UNIQUAC). The expressions of H_m^E derived from the G^E model were developed through the Gibbs–Helmholtz equation

Table 3. Excess Molar Enthalpies of the System Acetophenone (1) + 1-Propanol (2)

x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$	x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$	x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$
$T = 298.15$ K, $p = 0.1$ MPa					
0.0997	589.5	0.3998	1313.3	0.6004	1336.1
0.2003	952.1	0.4501	1349.1	0.7003	1218.1
0.3002	1177.6	0.5003	1364.4	0.8006	991.3
0.3505	1257.3	0.5499	1362.1	0.9002	601.5
$T = 313.15$ K, $p = 0.1$ MPa					
0.0997	660.3	0.3998	1525.7	0.6004	1531.1
0.2003	1091.3	0.4501	1565.1	0.7003	1373.2
0.3002	1368.2	0.5003	1579.1	0.8006	1082.5
0.3505	1462.7	0.5499	1569.0	0.9002	630.7
$T = 328.15$ K, $p = 0.1$ MPa					
0.0997	728.7	0.3998	1745.0	0.6004	1741.9
0.2003	1233.9	0.4501	1789.3	0.7003	1551.0
0.3002	1565.0	0.5003	1806.2	0.8006	1207.3
0.3505	1672.6	0.5499	1786.3	0.9002	694.4
$T = 338.15$ K, $p = 0.1$ MPa					
0.0997	784.7	0.3998	1846.7	0.6004	1821.9
0.2003	1316.2	0.4501	1889.5	0.7003	1607.7
0.3002	1655.7	0.5003	1899.9	0.8006	1241.8
0.3505	1769.9	0.5499	1879.5	0.9002	705.3
$T = 348.15$ K, $p = 0.1$ MPa					
0.0997	802.9	0.3998	1904.2	0.6004	1867.3
0.2003	1354.7	0.4501	1946.3	0.7003	1639.4
0.3002	1714.3	0.5003	1954.3	0.8006	1258.6
0.3505	1827.9	0.5499	1928.7	0.9002	720.3

Table 4. Excess Molar Enthalpies of the System Acetophenone (1) + 2-Propanol (2)

x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$	x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$	x_1	$\frac{H_m^E}{J\cdot mol^{-1}}$
$T = 298.15$ K, $p = 0.1$ MPa					
0.1000	709.3	0.3995	1527.3	0.6003	1523.5
0.2001	1135.2	0.4497	1560.8	0.7006	1375.8
0.2996	1387.7	0.4996	1570.3	0.7994	1112.3
0.3502	1470.9	0.5503	1560.2	0.9005	673.3
$T = 313.15$ K, $p = 0.1$ MPa					
0.1000	823.2	0.3995	1798.1	0.6003	1772.3
0.2001	1321.9	0.4497	1835.6	0.7006	1582.3
0.2996	1634.8	0.4996	1843.3	0.7994	1246.7
0.3502	1732.8	0.5503	1823.4	0.9005	725.8
$T = 328.15$ K, $p = 0.1$ MPa					
0.1000	886.0	0.3995	1973.7	0.6003	1927.7
0.2001	1448.8	0.4497	2014.1	0.7006	1701.0
0.2996	1788.0	0.4996	2018.8	0.7994	1323.0
0.3502	1902.6	0.5503	1991.5	0.9005	751.6
$T = 338.15$ K, $p = 0.1$ MPa					
0.1000	888.0	0.3995	2025.9	0.6003	1972.4
0.2001	1477.0	0.4497	2066.3	0.7006	1732.6
0.2996	1833.8	0.4996	2070.3	0.7994	1337.5
0.3502	1952.0	0.5503	2037.5	0.9005	759.4
$T = 348.15$ K, $p = 0.1$ MPa					
0.1000	890.7	0.3995	2037.1	0.6003	1974.3
0.2001	1480.5	0.4497	2075.6	0.7006	1734.3
0.2996	1845.6	0.4996	2077.9	0.7994	1342.2
0.3502	1962.1	0.5503	2044.9	0.9005	762.5

$$\left[\frac{\partial(G_m^E/T)}{\partial T}\right]_{P,x} = -\frac{H_m^E}{T^2} \tag{2}$$

Redlich–Kister Equation. The Redlich–Kister equation[8] is commonly used to correlate H_m^E data because of its simplicity

$$H_m^E = x_1(1 - x_1)\sum_{i=0}^{n} A_i(2x_1 - 1)^i \tag{3}$$

where x_1 is the mole fraction of acetophenone; A_i is the adjustable parameter; and n is the number of fitted parameters.

The Redlich–Kister parameters were obtained by the least-squared fit method, which were listed in Table 5 together with the root-mean-square deviations (σ). The σ is defined as

$$\sigma = \sqrt{\frac{1}{N}\sum_{i}^{N}(H^{\mathrm{E}}_{\mathrm{calcd}(i)} - H^{\mathrm{E}}_{\mathrm{exptl}(i)})^2} \qquad (4)$$

where $H^{\mathrm{E}}_{\mathrm{calcd}(i)}$ and $H^{\mathrm{E}}_{\mathrm{exptl}(i)}$ are the calculated values and experimental values of excess molar enthalpies and N is the number of data for each data set.

Wilson Model. The expression of $H^{\mathrm{E}}_{\mathrm{m}}$ derived from the Wilson G^{E} model[9] is given in eq 5

$$H^{\mathrm{E}}_{\mathrm{m}} = x_1\left(\frac{\Lambda_{21}x_2}{x_1 + \Lambda_{21}x_2}\right)(\lambda_{21} - \lambda_{22}) + x_2\left(\frac{\Lambda_{12}x_1}{x_2 + \Lambda_{12}x_1}\right)(\lambda_{12} - \lambda_{11}) \qquad (5)$$

with

$$\Lambda_{12} = \frac{V_{\mathrm{m}1}}{V_{\mathrm{m}2}}\exp[-(\lambda_{12} - \lambda_{11})/RT],$$
$$\Lambda_{21} = \frac{V_{\mathrm{m}2}}{V_{\mathrm{m}1}}\exp[-(\lambda_{21} - \lambda_{22})/RT],$$

where $V_{\mathrm{m},i}$ is the molar volume of pure component i (see Table S2 in the Supporting Information) and λ_{ij} and λ_{ii} are the interaction energy parameters. The parameters ($\lambda_{ij} - \lambda_{ii}$) of the Wilson equation are obtained by a nonlinear least-squares fit and listed in Table 6 together with σ.

NRTL Model. The expression of $H^{\mathrm{E}}_{\mathrm{m}}$ derived from the NRTL G^{E} model[10] is given in eq 6

$$H^{\mathrm{E}}_{\mathrm{m}} = x_1x_2\left[\frac{G_{21}(g_{21} - g_{11})(x_1 + x_2G_{21} - x_1\tau_{21}\alpha_{21})}{(x_1 + x_2G_{21})^2} + \frac{G_{12}(g_{12} - g_{22})(x_2 + x_1G_{12} - x_2\tau_{12}\alpha_{12})}{(x_2 + x_1G_{12})^2}\right] \qquad (6)$$

with

$$\tau_{21} = (g_{21} - g_{11})/RT, \quad \tau_{12} = (g_{12} - g_{22})/RT$$
$$G_{12} = \exp(-\alpha_{12}\tau_{12}), \quad G_{21} = \exp(-\alpha_{12}\tau_{21})$$

where ($g_{21} - g_{11}$) and ($g_{12} - g_{22}$) are the interaction energy parameters and α_{12} is the nonrandomness parameter. They are obtained by a nonlinear least-squares fit. The parameters of the NRTL equation and σ are listed in Table 7.

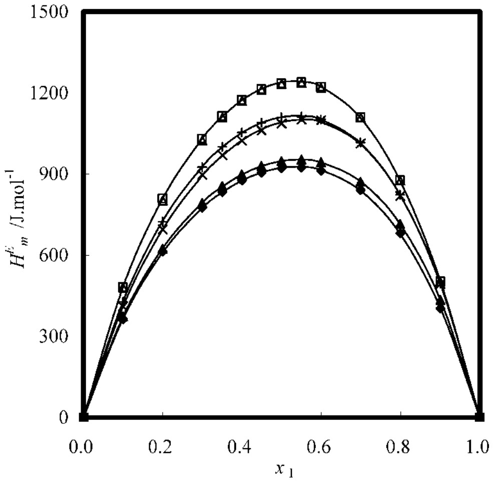

Figure 1. Excess molar enthalpies of the system acetophenone (1) + methanol (2) as a function of mole fraction x_1. ◆, 298.15 K, 0.1 MPa; ▲, 298.15 K, 10.0 MPa; ×, 313.15 K, 0.1 MPa; +, 313.15 K, 10.0 MPa; Δ, 328.15 K, 0.1 MPa; □, 328.15 K, 10.0 MPa. The curves were calculated by the Redlich–Kister equation (parameters taken from Table 5).

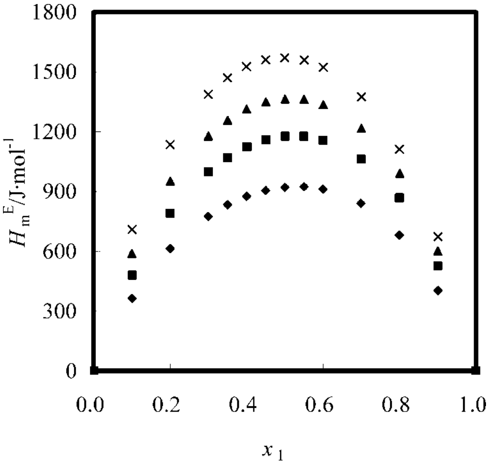

Figure 2. Excess molar enthalpies for the system acetophenone (1) + alcohols (2) as a function of mole fraction x_1 at 298.15 K and 0.1 MPa. ◆, acetophenone (1) + methanol (2); □, acetophenone (1) + aethanol (2); ▲, acetophenone (1) + 1-propanol (2); ×, acetophenone (1) + 2-propanol (2).

UNIQUAC Model. From the UNIQUAC G^{E} model,[11] $H^{\mathrm{E}}_{\mathrm{m}}$ can be derived as follows

$$H^{\mathrm{E}}_{\mathrm{m}} = q_1x_1\left(\frac{\theta_2}{\theta_1 + \theta_2\tau_{21}}\right)\tau_{21}\Delta u_{21} + q_2x_2\left(\frac{\theta_1}{\theta_2 + \theta_1\tau_{12}}\right)\tau_{12}\Delta u_{12} \qquad (7)$$

with

Table 5. Parameters A_i of the Redlich–Kister Equation with the Root-Mean-Square Deviation (σ)

		Redlich–Kister Equation				
T / K	p / MPa	A_0 / J·mol^{-1}	A_1 / J·mol^{-1}	A_2 / J·mol^{-1}	A_3 / J·mol^{-1}	σ / J·mol^{-1}
		Acetophenone (1) + Methanol (2)				
298.15	0.1	3693.6	406.9	919.4	−191.5	1.8
	10.0	3792.6	469.1	1097.9	−66.1	1.1
313.15	0.1	4368.8	716.9	1031.4	−211.1	3.3
	10.0	4444.7	514.8	1088.1	−89.5	1.9
328.15	0.1	4942.7	582.1	821.8	−651.1	2.3
	10.0	4956.7	538.0	835.0	−607.7	1.8
		Acetophenone (1) + Ethanol (2)				
298.15	0.1	4696.1	412.1	1390.4	−101.1	2.4
	10.0	4704.5	479.6	1540.5	−101.1	3.0
313.15	0.1	5582.4	509.4	1410	−211.3	2.7
	10.0	5587.6	510.7	1418.8	−224.6	2.6
328.15	0.1	6264.4	334.9	988.8	−301.8	1.4
	10.0	6271.3	370.59	1045.9	−310.1	2.0
338.15	0.1	6679	150.3	897.1	−561.8	2.0
	10.0	6684.6	156.5	928.0	−559.1	2.4
		Acetophenone (1) + 1-Propanol (2)				
298.15	0.1	5441.4	314.8	1827.4	−353.7	4.2
313.15	0.1	6351.8	125.0	1355.4	−510.1	1.9
328.15	0.1	7226.9	−10.0	1102.7	−356.1	2.5
338.15	0.1	7602.0	−182.0	1087.2	−574.8	1.5
348.15	0.1	7816.7	−373.9	1026.2	−317.9	1.3
		Acetophenone (1) + 2-Propanol (2)				
298.15	0.1	6260.8	−8.8	2200.4	−343.8	4.6
313.15	0.1	7361.3	−177.6	1935.3	−727.4	3.8
328.15	0.1	8067.8	−396.5	1630.3	−793.0	2.2
338.15	0.1	8277.5	−536.5	1398.4	−523.3	1.2
348.15	0.1	8307.8	−592.9	1398	−420.6	1.2

Table 6. Parameters of the Wilson Equation with the Root-Mean-Square Deviation (σ)

	Wilson		
p / MPa	$(\lambda_{12} - \lambda_{11})$ / $\mathrm{J \cdot mol^{-1}}$	$(\lambda_{21} - \lambda_{22})$ / $\mathrm{J \cdot mol^{-1}}$	σ / $\mathrm{J \cdot mol^{-1}}$
	Acetophenone (1) + Methanol (2)		
0.1	4321.27	3096.45	163.8
10.0	4310.09	3088.83	170.6
	Acetophenone (1) + Ethanol (2)		
0.1	4019.54	3291.79	537.3
10.0	4029.78	3287.16	537.6
	Acetophenone (1) + 1-Propanol (2)		
0.1	3887.45	3475.64	788.6
	Acetophenone (1) + 2-Propanol (2)		
0.1	3847.62	3488.62	958.1

Table 7. Parameters of the NRTL Equation with the Root-Mean-Square Deviation (σ)

	NRTL			
p / MPa	$(g_{12} - g_{22})$ / $\mathrm{J \cdot mol^{-1}}$	$(g_{21} - g_{11})$ / $\mathrm{J \cdot mol^{-1}}$	α_{12}	σ / $\mathrm{J \cdot mol^{-1}}$
	Acetophenone (1) + Methanol (2)			
0.1	5973.20	4947.26	0.311	68.7
10.0	5906.60	4948.75	0.307	59.7
	Acetophenone (1) + Ethanol (2)			
0.1	7766.96	7218.48	0.237	90.9
10.0	7845.77	7235.46	0.236	89.2
	Acetophenone (1) + 1-Propanol (2)			
0.1	8474.29	8912.77	0.205	98.1
	Acetophenone (1) + 2-Propanol (2)			
0.1	8320.83	9525.04	0.185	78.0

Table 8. Parameters of the UNIQUAC Equation with the Root-Mean-Square Deviation (σ)

	UNIQUAC		
p / MPa	Δu_{21} / $\mathrm{J \cdot mol^{-1}}$	Δu_{12} / $\mathrm{J \cdot mol^{-1}}$	σ / $\mathrm{J \cdot mol^{-1}}$
	Acetophenone (1) + Methanol (2)		
0.1	221.97	3644.64	81.6
10.0	262.67	3628.21	73.3
	Acetophenone (1) + Ethanol (2)		
0.1	685.59	3134.10	120.4
10.0	685.59	3169.61	119.3
	Acetophenone (1) + 1-Propanol (2)		
0.1	1137.07	2347.48	145.5
	Acetophenone (1) + 2-Propanol (2)		
0.1	1679.86	2422.36	115.1

$$\tau_{21} = \exp(-\Delta u_{21}/RT), \quad \tau_{12} = \exp(-\Delta u_{12}/RT)$$

$$\theta_1 = x_1 q_1/(x_1 q_1 + x_2 q_2), \quad \theta_2 = x_2 q_2/(x_1 q_1 + x_2 q_2),$$

where q_i is the structural parameter of the pure component (see Table S4 in the Supporting Information); Δu_{12} and Δu_{21} are the interaction energy parameters, which are obtained by a nonlinear least-squares fit. They are given in Table 8 together with σ.

From Tables 1 to 4, it can be seen that the mixing processes for all binary systems in this work show endothermic behavior. The positive value of H_m^E indicates that acetophenone can not easily interact with alcohols to form crossed associations through the intermolecular hydrogen bond. From Figure 1, H_m^E values increase with an increase of temperature and pressure. The effect of temperature on excess molar enthalpies is much more distinct than pressure. From Figure 2, it can be seen that the H_m^E value increases with the increasing of branch and carbon number of alcohols. It may be due to the increasing difficulty to form crossed associations between acetophenone and alcohols with increasing steric hindrance and aliphatic chain of alcohol.

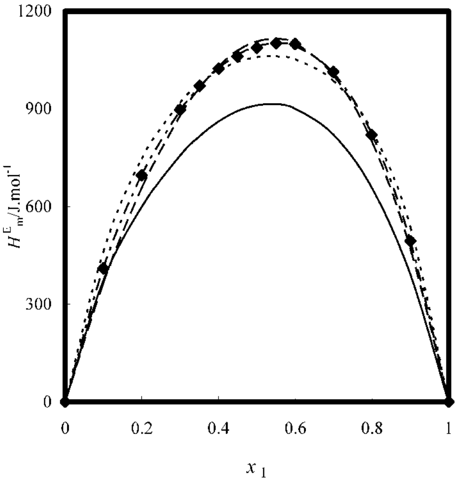

Figure 3. Correlation of excess molar enthalpies of the system acetophenone (1) + methanol (2) as a function of mole fraction x_1. ◆, experiment data at 313.15 K and 0.1 MPa; -•-, calculated by the Redlich–Kister equation (parameters taken from Table 5); —, calculated by the Wilson equation (parameters taken from Table 6); •••••, calculated by the NRTL equation (parameters taken from Table 7); - -, calculated by the UNIQUAC equation (parameters taken from Table 8).

From Tables 5 to 8, it can be seen that the Redlich–Kister equation and the NRTL and UNIQUAC models can give a good correlation of the excess molar enthalpies for the systems in this work, while the Wilson model has an obvious deviation. The σ values for the correlating results show the temperature has some effect on parameters. As a typical example, the correlation curves for excess molar enthalpies of acetophenone (1) + methanol (2) at 313.15 K and 0.1 MPa are plotted in Figure 3.

Supporting Information Available:

Tables S1 to S4. This material is available free of charge via the Internet at http://pubs.acs.org.

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